Supporting Information

Synthesis and Characterization of $Os^{IV}(acac)_2PhCl$ and Demonstation of H/D Exchange in Benzene.

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Spectral Data:

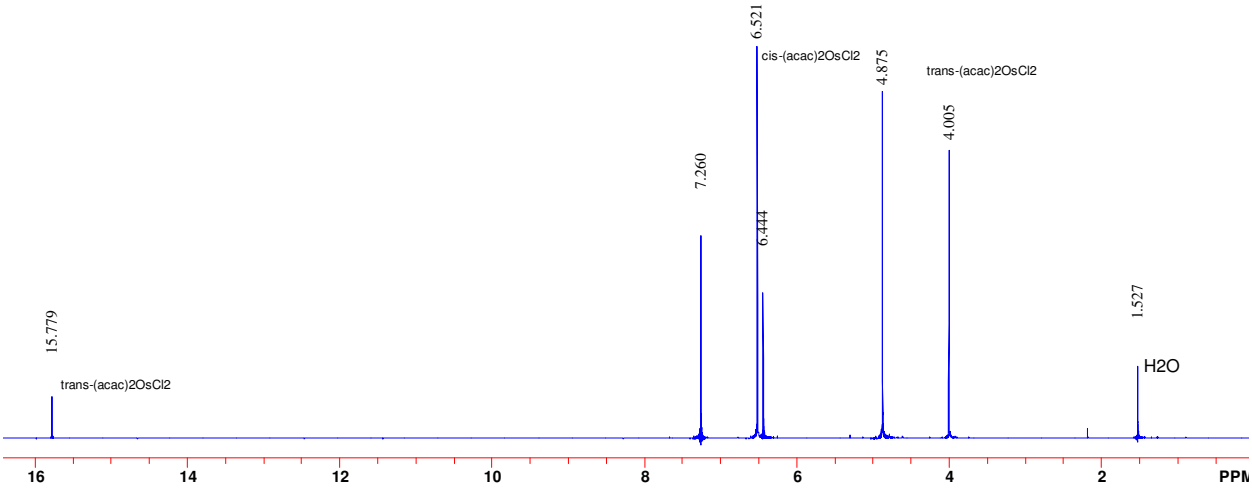


Figure S1. ^{1}H NMR of cis and trans-$(acac)_2OsCl_2$.

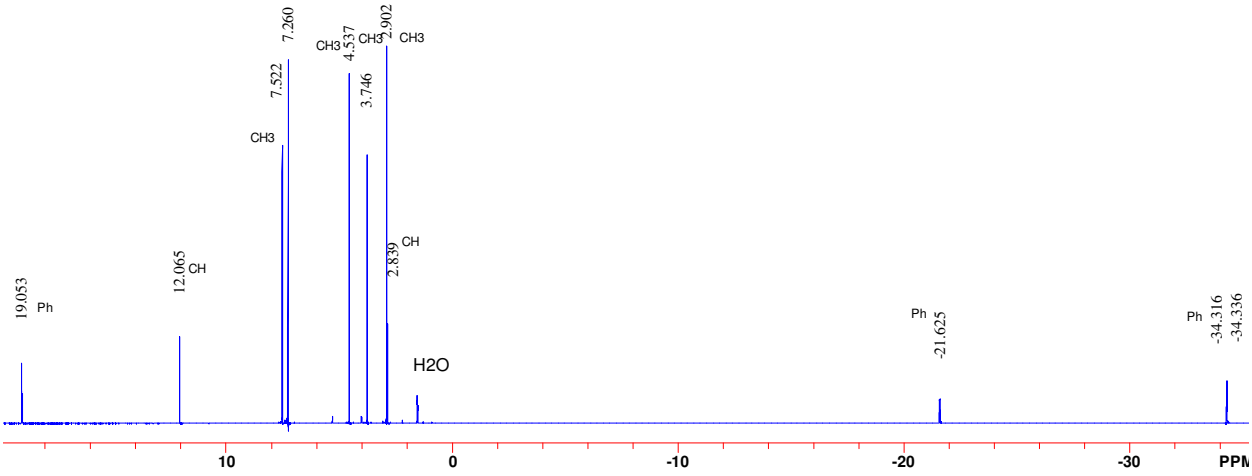


Figure S2. ^{1}H NMR of cis-$(acac)_2OsPhCl$.

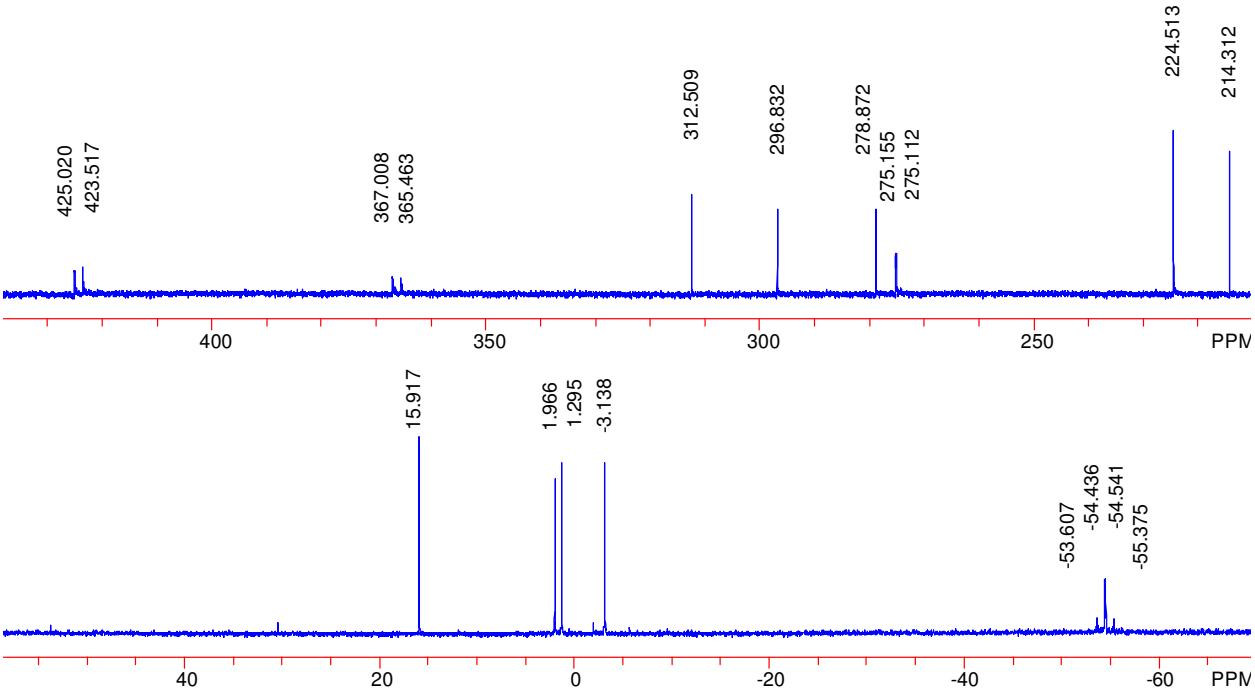
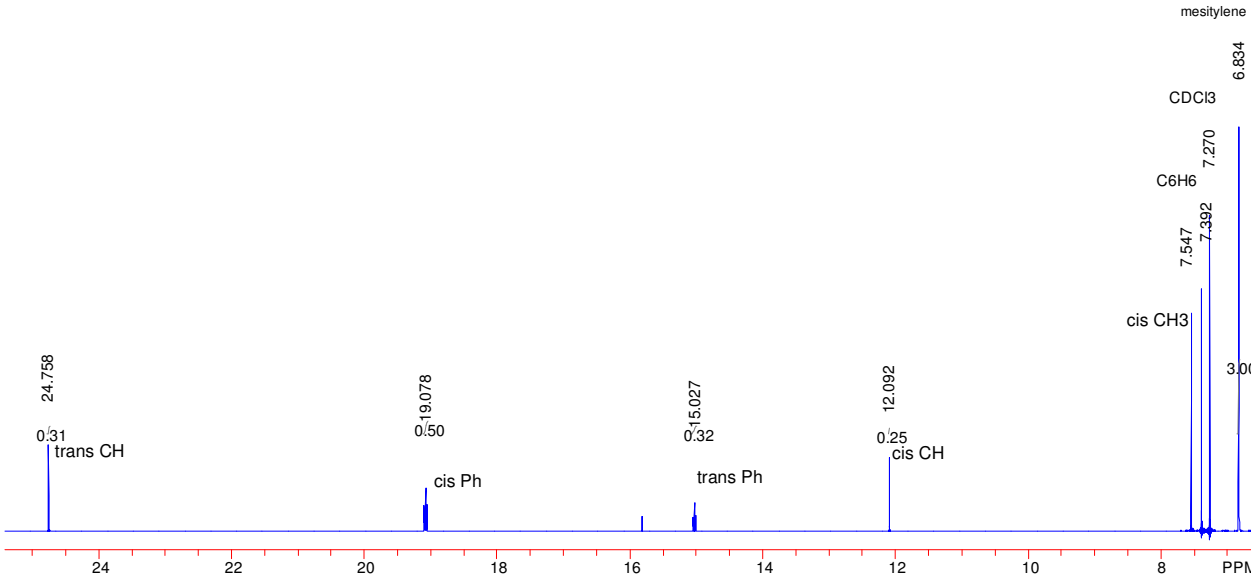


Figure S3. ^{13}C NMR of cis-$(acac)_2OsPhCl$.



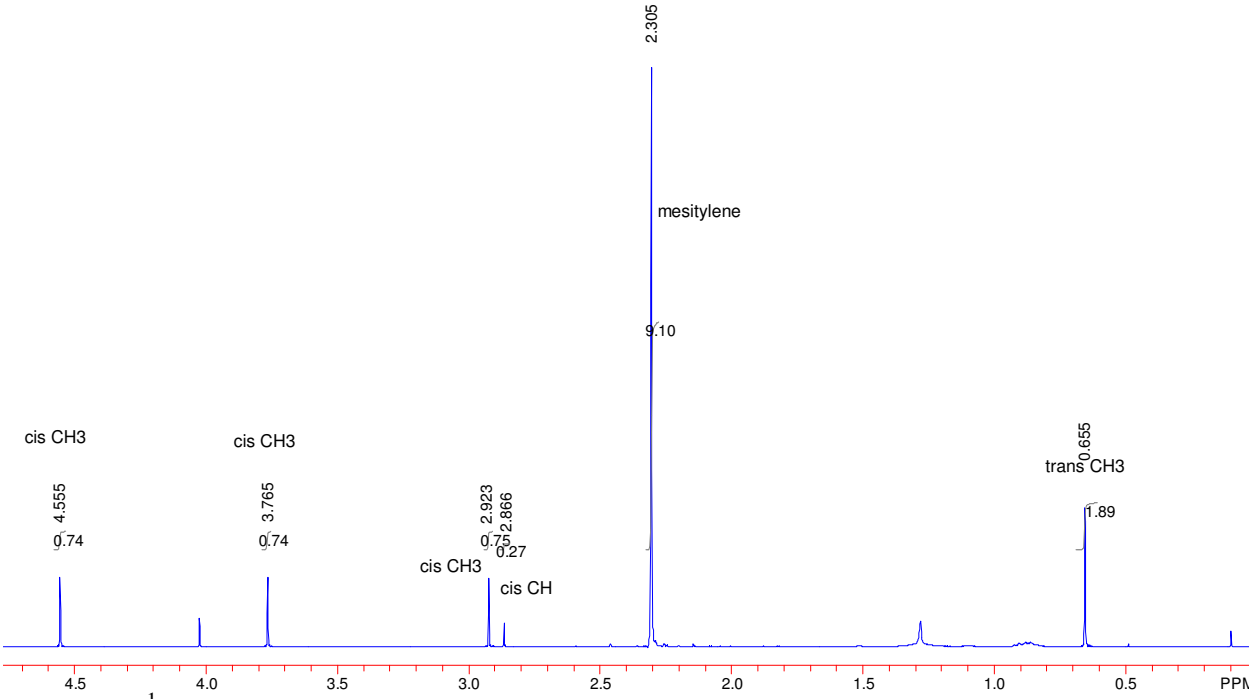


Figure S4. ^{1}H NMR of the reaction mixture after thermolysis of cis-1Ph in C_6H_6. Top expansion of 25-7ppm range. Bottom expansion of 5-0ppm range.

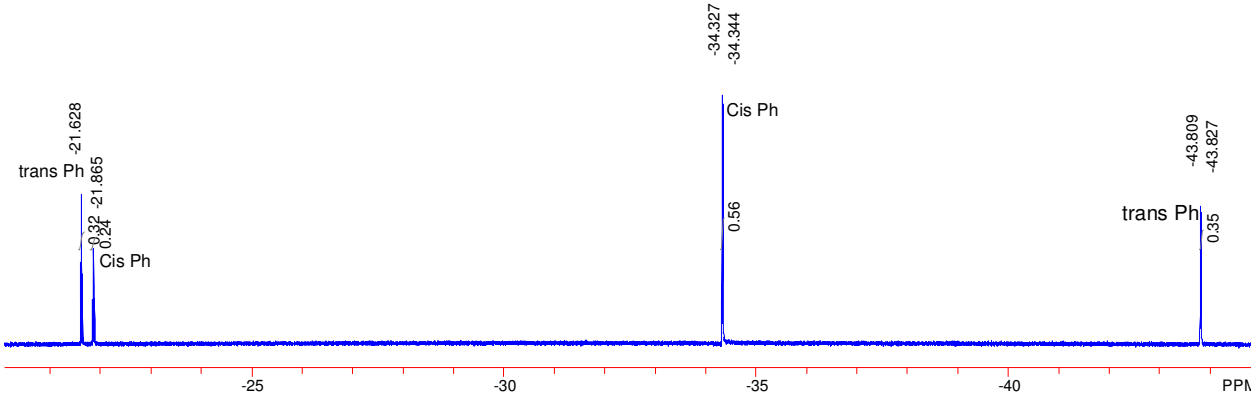


Figure S5. ^{1}H NMR of the reaction mixture after thermolysis of cis-1Ph in C_6H_6 continued, expansion of -20 to -45 ppm range.

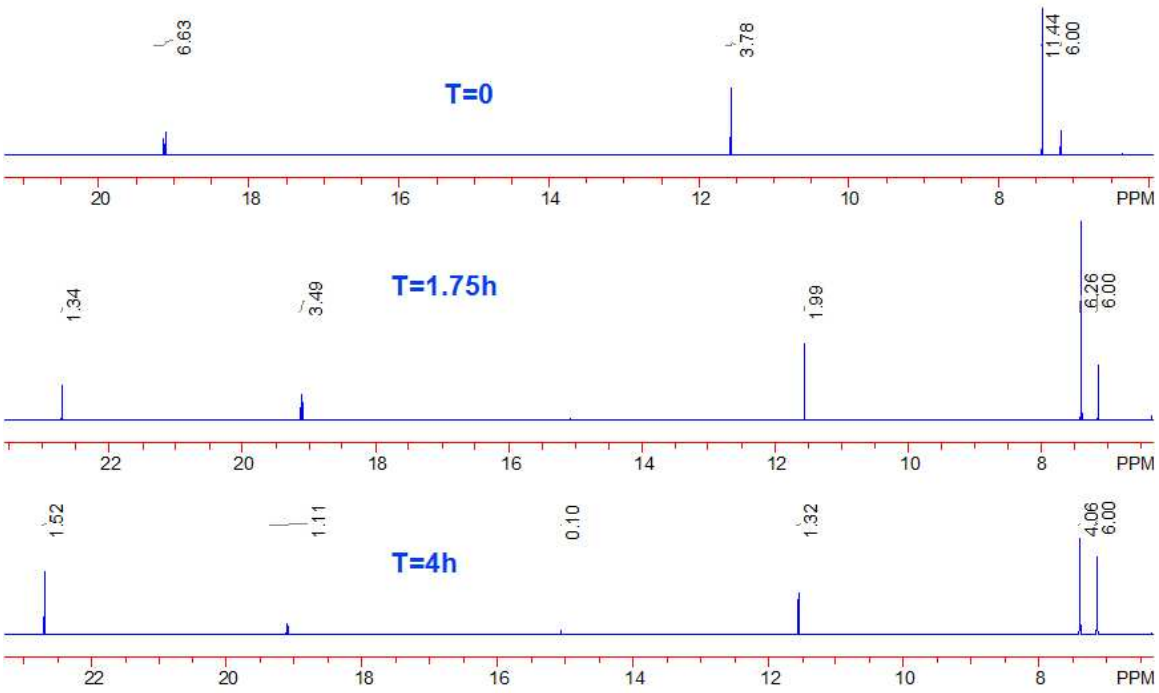


Figure S6. ^{1}H NMR after heating cis-1Ph in C_6D_6, expansion of -23 to -7 ppm range.

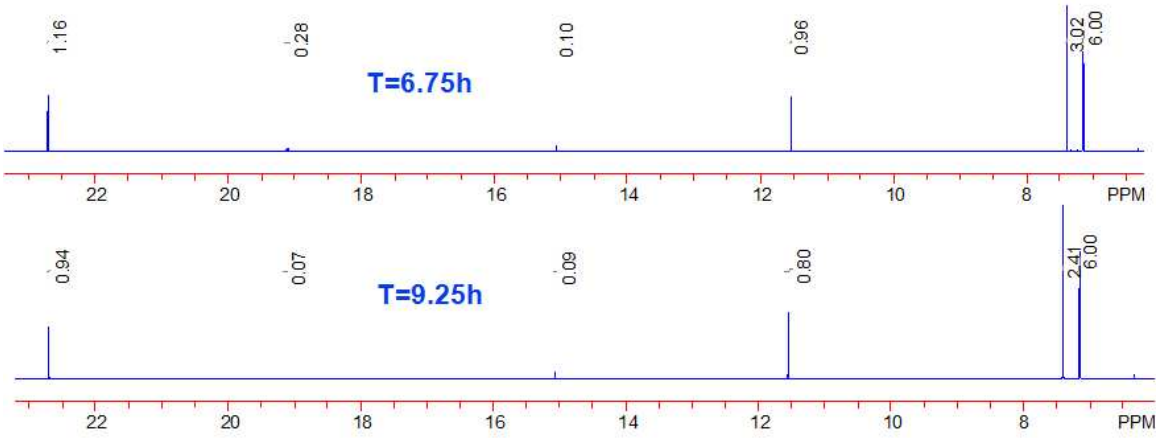


Figure S7. ^{1}H NMR after heating cis-1Ph in C_6D_6 continued, expansion of -23 to -7 ppm range.

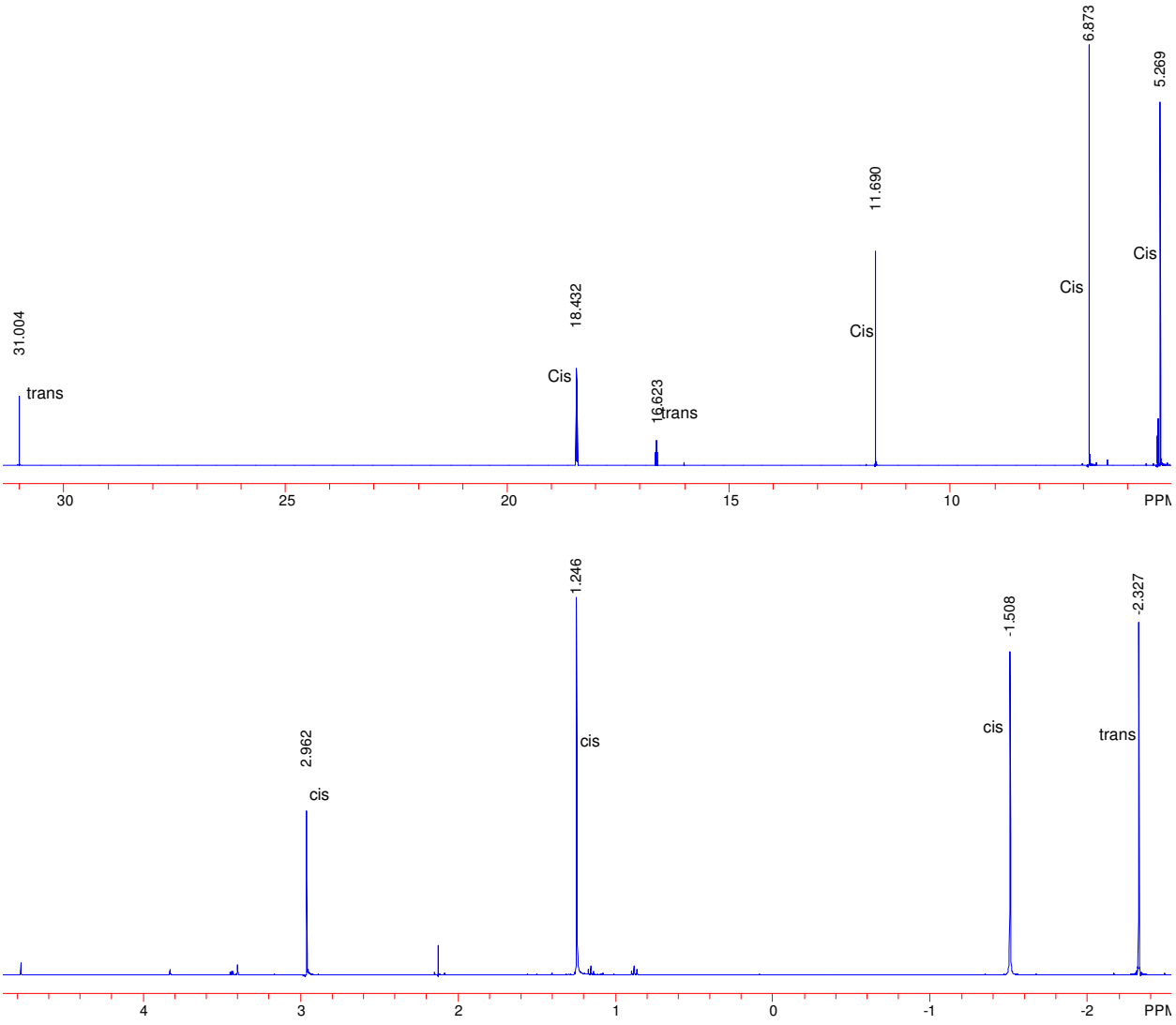


Figure S8. ^{1}H NMR of the crude reaction mixture after treatment of cis-1Ph with AgOTf. Top expansion of 32-5ppm range. Bottom expansion of 5-3ppm range.

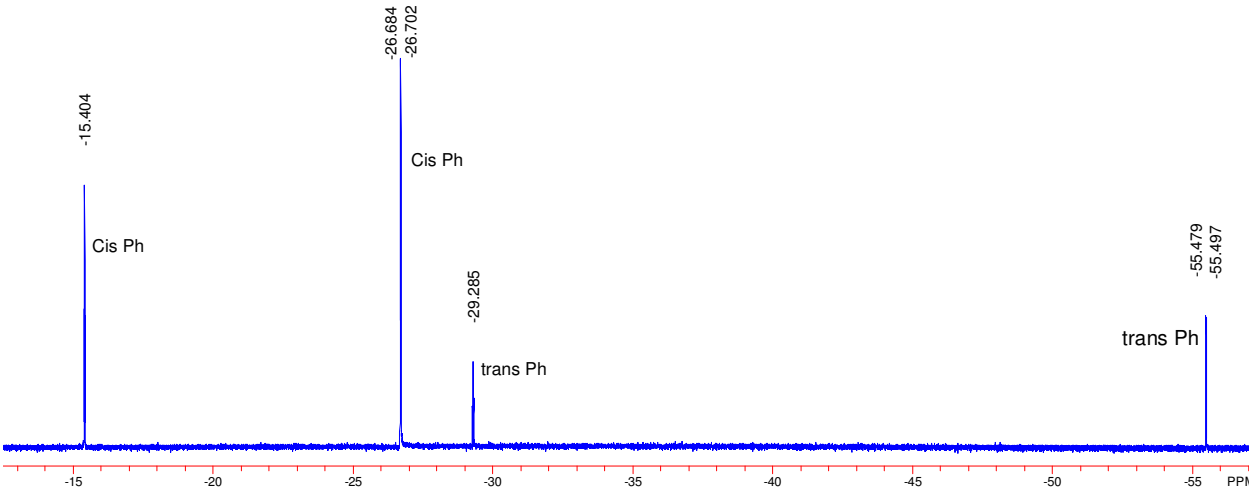


Figure S9. ^{1}H NMR of the crude reaction mixture after treatment of cis-1Ph with AgOTf, continued, expansion of -12 to -57 ppm range.

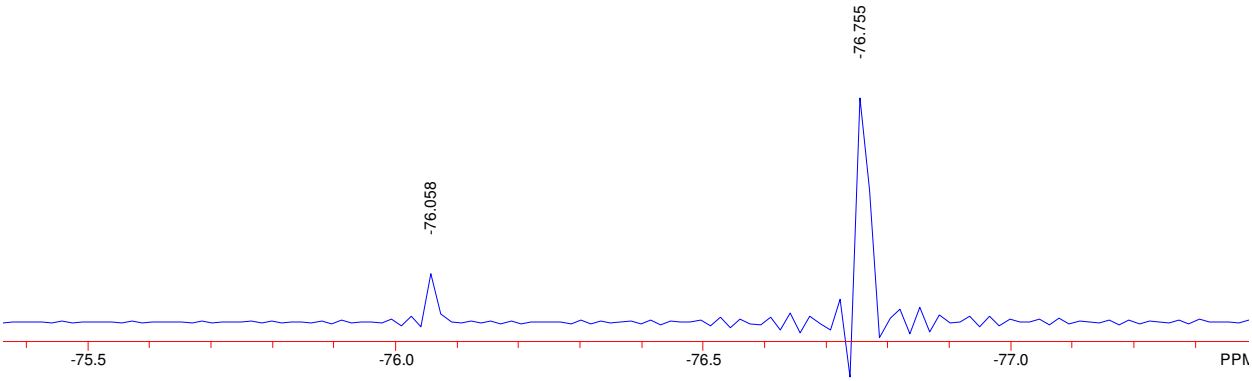


Figure S10. ^{19}F NMR of the crude reaction mixture after treatment of cis-1Ph with AgOTf.

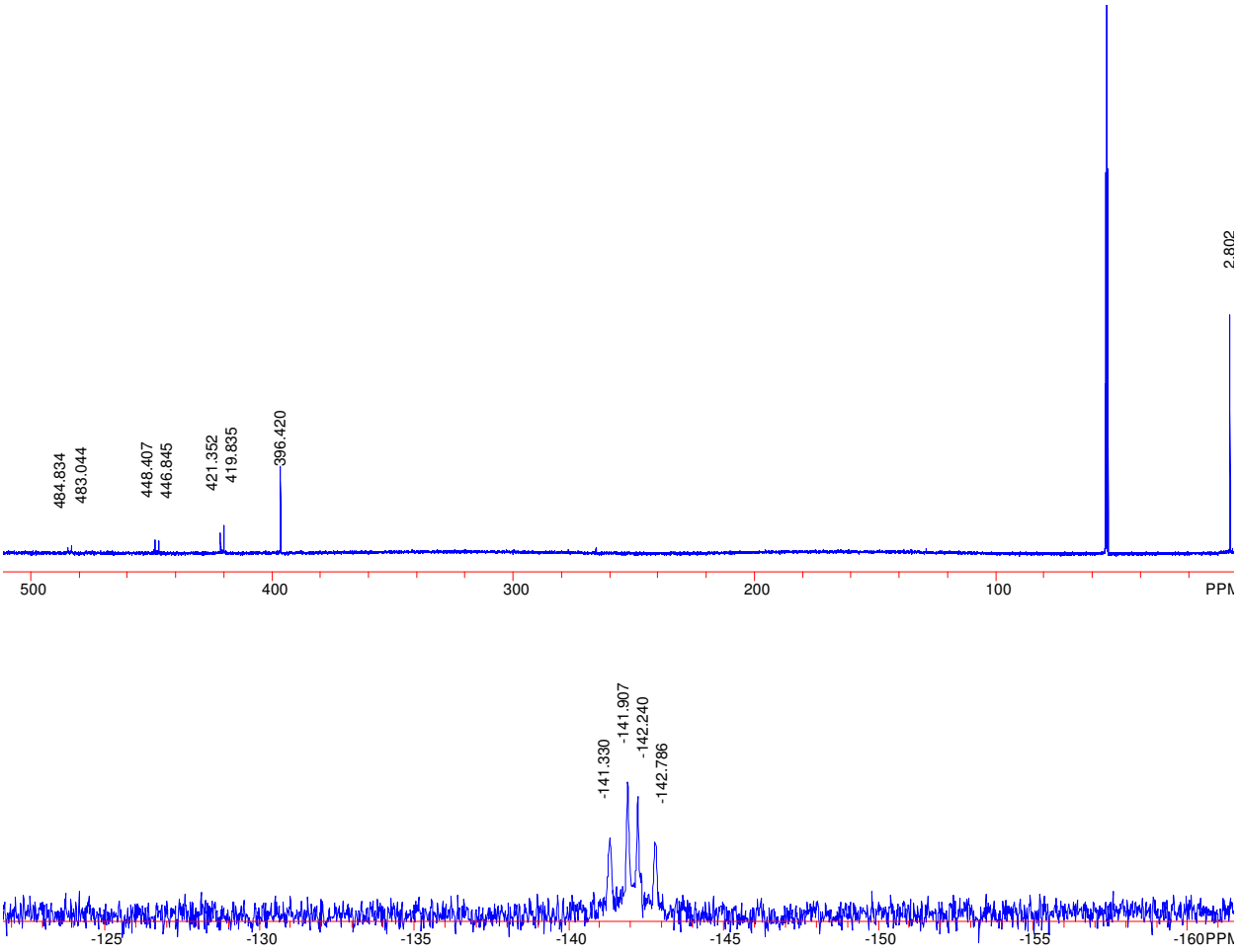


Figure S11. ^{13}C NMR of the trans-OTf-1-Ph.

H/D exchange benzene/toluene-d8 no Zinc

time	H6	d1	d2	d3	d4	d5	d6	
0	100	0.00	0	0	0	0	0	
6	99.79	0.00	0.10	0.07	0.03	0.01	0.01	
16.5	37.31	11.70	12.86	12.77	12.16	9.10	4.11	
16.5	37.84	12.03	13.15	12.84	11.67	8.64	3.84	
22.5	28.24	12.12	14.09	14.97	14.61	11.09	4.88	
22.5	28.56	12.10	13.98	14.90	14.44	11.09	4.93	
39.5	22.42	11.26	13.95	16.02	16.69	13.67	6.00	
39.5	22.48	11.46	13.84	15.91	16.72	13.63	5.95	

H/D exchange benzene/toluene-d8 with Zinc

time	H6	d1	d2	d3	d4	d5	d6
3.1	79.08	4.53	4.98	4.14	3.47	2.56	1.25
3.1	79.00	4.55	4.99	4.15	3.46	2.55	1.28
6.1	71.16	6.32	6.56	5.65	4.80	3.67	1.85

6.1	71.12	6.32	6.60	5.62	4.81	3.68	1.85
10.1	66.68	7.26	7.40	6.53	5.58	4.32	2.22
10.1	66.29	7.29	7.44	6.52	5.71	4.48	2.27
22.0	62.46	7.93	8.29	7.34	6.40	5.01	2.58
22.0	63.04	8.10	8.28	7.23	6.21	4.73	2.41

H/D exchange benzene/toluene-d8 with HgPh2

time	H6	d1	d2	d3	d4	d5	d6
6	82.48	3.59	4.32	3.5	2.93	2.12	1.06
16.5	81.74	3.92	4.4	3.65	2.96	2.19	1.13
22.5	80.51	4.38	4.6	3.83	3.13	2.35	1.2

H/D exchange benzene/toluene-d8 diluted

time	H6	d1	d2	d3	d4	d5	d6
5	99.9	0	0.01	0.04	0.02	0.01	0.01
18.2	98.12	0	0.69	0.51	0.36	0.23	0.1
18.2	98.09	0	0.69	0.52	0.37	0.23	0.1
41.8	95.85	0.32	1.38	1	0.74	0.49	0.22
41.8	95.63	0.44	1.39	1.03	0.78	0.51	0.22
88.3	93.51	1.11	1.79	1.44	1.09	0.73	0.34
88.3	93.15	1.29	1.85	1.45	1.13	0.78	0.36

Reduction of cis-$(acac)_2OsCl_2$: A J-Young NMR tube was loaded with 5mg of cis-$(acac)_2OsCl_2$ and NCCD3 (0.7mL). To this red solution excess Na/Hg amalgam was added. The solution turned dark purple red and after 1h it turned dark yellow. ^{1}H NMR analysis shows a potential Os(III) intermediate (broad peaks at 1.11 and 0.99ppm), as well as the cis and trans Os(II) complex.

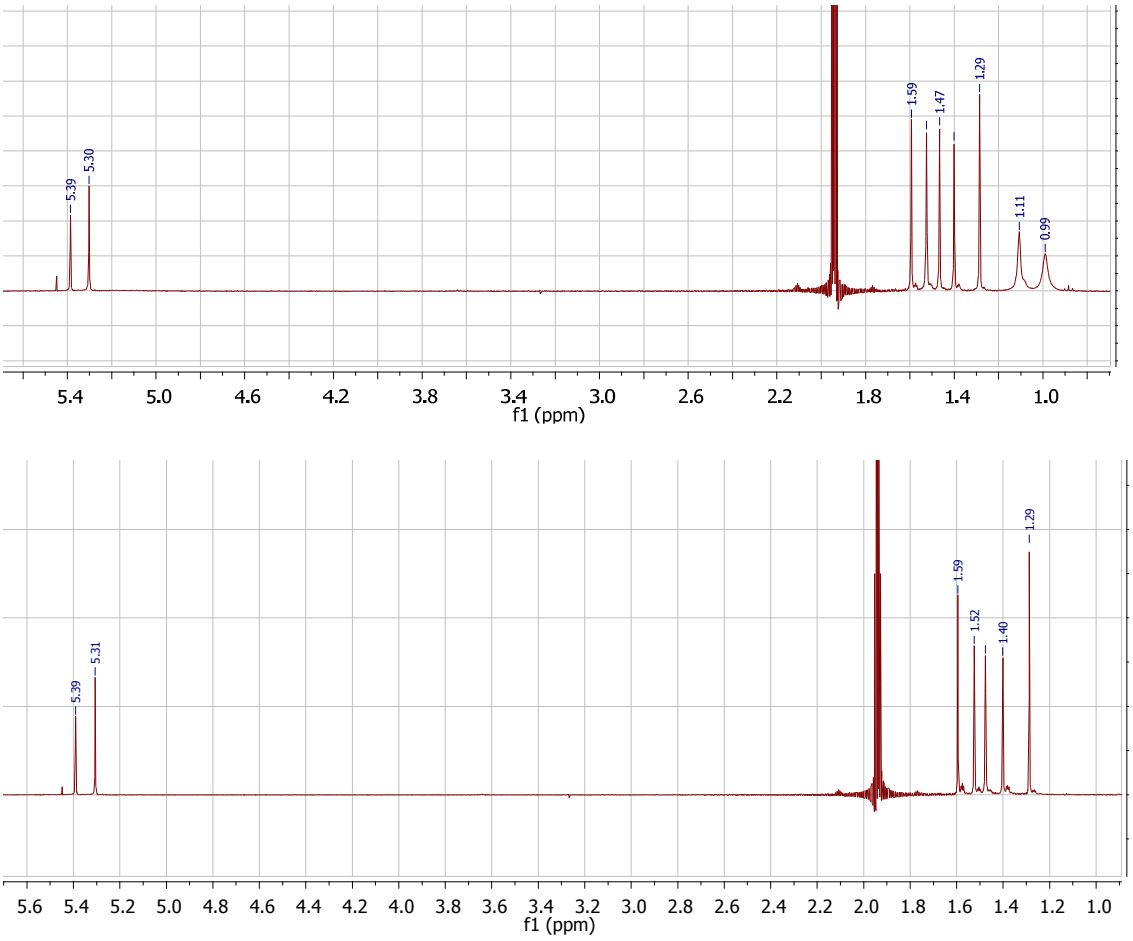


Figure S12. Top: ^{1}H NMR of cis-$(acac)_2OsCl_2$ + Na/Hg after ~15min. Bottom ^{1}H NMR after 1h.

Table 1. Crystal data and structure refinement for **Trans-OTf-1-Ph**.

Identification code	osphotfm	
Empirical formula	C17 H19 F3 O7 Os S	
Formula weight	614.58	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.5774(6) Å	α= 86.170(2)°.
	b = 9.3032(5) Å	β= 88.963(3)°.
	c = 13.0773(7) Å	γ = 85.364(3)°.
Volume	1037.71(11) $Å^3$	
Z	2	
Density (calculated)	1.967 Mg/m^3	
Absorption coefficient	6.306 mm^{-1}	
F(000)	592	
Crystal size	0.50 x 0.05 x 0.01 mm^3	
Theta range for data collection	2.78 to 27.45°.	
Index ranges	-10<=h<= 7, -12<=k<=9, -16<=l<=16	
Reflections collected	6338	
Independent reflections	4455 [R(int) = 0.0241]	
Completeness to theta = 27.45°	93.8 %	
Transmission factors	min/max ratio: 0.491	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4455 / 15 / 264	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0372, wR2 = 0.0828	
R indices (all data)	R1 = 0.0459, wR2 = 0.0859	
Largest diff. peak and hole	1.529 and -1.327 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Trans-OTf-1-Ph**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Os1	0.10493(2)	0.67010(2)	0.252268(16)	0.01960(8)
S1	0.35626(16)	0.35805(16)	0.25328(11)	0.0252(3)
F1	0.109(5)	0.263(5)	0.193(5)	0.080(9)
F2	0.171(4)	0.190(5)	0.347(5)	0.087(7)
F3	0.293(6)	0.097(3)	0.221(5)	0.071(8)
F1	0.122(3)	0.259(3)	0.1589(16)	0.066(4)
F2A	0.1771(17)	0.151(2)	0.305(2)	0.074(5)
F3A	0.3235(19)	0.1128(16)	0.174(2)	0.065(4)
O1	0.2598(4)	0.7211(4)	0.1444(3)	0.0231(8)
O2	0.2237(4)	0.7609(4)	0.3550(3)	0.0266(9)
O3	-0.0040(4)	0.5710(4)	0.1504(3)	0.0228(8)
O4	-0.0393(4)	0.6054(4)	0.3617(3)	0.0243(8)
O5	0.2470(5)	0.4662(4)	0.2974(3)	0.0310(9)
O6	0.4675(5)	0.2931(5)	0.3251(3)	0.0420(12)
O7	0.4154(5)	0.4032(5)	0.1541(3)	0.0416(11)
C1	0.5014(7)	0.7646(7)	0.0666(5)	0.0329(14)
C2	0.3990(6)	0.7573(6)	0.1598(4)	0.0229(12)
C3	0.4522(7)	0.7925(7)	0.2542(4)	0.0288(13)
C4	0.3642(7)	0.8001(6)	0.3436(4)	0.0262(13)
C5	0.4281(8)	0.8574(8)	0.4363(5)	0.0395(16)
C6	-0.1977(7)	0.4592(7)	0.0682(4)	0.0298(13)
C7	-0.1380(6)	0.5163(6)	0.1629(4)	0.0224(12)
C8	-0.2191(7)	0.5055(7)	0.2561(4)	0.0288(13)
C9	-0.1675(6)	0.5446(6)	0.3493(4)	0.0260(13)
C10	-0.2593(7)	0.5161(8)	0.4459(4)	0.0378(16)
C11	-0.0378(6)	0.8509(6)	0.2217(4)	0.0248(12)
C12	-0.0766(7)	0.8979(7)	0.1218(5)	0.0299(13)
C13	-0.1805(7)	1.0190(7)	0.1004(5)	0.0371(15)
C14	-0.2480(7)	1.0933(7)	0.1815(6)	0.0409(17)
C15	-0.2098(7)	1.0481(7)	0.2806(5)	0.0351(15)
C16	-0.1056(7)	0.9287(7)	0.3026(5)	0.0330(14)
C17	0.2326(9)	0.2135(8)	0.2295(7)	0.054(2)

Table 3. Bond lengths [Å] and angles [°] for **Trans-OTf-1-Ph**.

Os1- O3	1.961(3)	O2 C4	1.290(7)
Os1 O4	1.970(4)	O3 C7	1.297(6)
Os1 O2	1.974(4)	O4 C9	1.293(7)
Os1 O1	1.981(4)	C1 C2	1.490(8)
Os1 C11	2.021(5)	C2 C3	1.391(7)
Os1 O5	2.221(4)	C3 C4	1.383(8)
S1 O6	1.421(4)	C4 C5	1.487(8)
S1 O7	1.433(5)	C6 C7	1.493(7)
S1 O5	1.460(4)	C7 C8	1.395(8)
S1 C17	1.824(7)	C8 C9	1.385(8)
F1 C17	1.21(3)	C9 C10	1.497(8)
F2 C17	1.63(5)	C11 C12	1.387(8)
F3 C17	1.17(3)	C11 C16	1.412(8)
F1A C17	1.361(17)	C12 C13	1.394(8)
F2A C17	1.221(19)	C13 C14	1.396(9)
F3A C17	1.399(19)	C14 C15	1.373(9)
O1 C2	1.290(6)	C15 C16	1.386(8)

O3 Os1 O4 91.27(15) .	C2 O1 Os1 125.7(3) .
O3 Os1 O2 176.81(15) .	C4 O2 Os1 126.0(4) .
O4 Os1 O2 89.38(16) .	C7 O3 Os1 126.4(4) .
O3 Os1 O1 88.49(15) .	C9 O4 Os1 126.2(3) .
O4 Os1 O1 175.64(15) .	S1 O5 Os1 140.4(2) .
O2 Os1 O1 90.63(16) .	O1 C2 C3 124.2(5) .
O3 Os1 C11 89.97(19) .	O1 C2 C1 114.8(5) .
O4 Os1 C11 90.35(19) .	C3 C2 C1 121.0(5) .
O2 Os1 C11 93.14(19) .	C4 C3 C2 125.9(6) .
O1 Os1 C11 94.01(19) .	O2 C4 C3 124.8(5) .
O3 Os1 O5 90.40(15) .	O2 C4 C5 114.4(5) .
O4 Os1 O5 84.46(15) .	C3 C4 C5 120.9(6) .
O2 Os1 O5 86.55(15) .	O3 C7 C8 124.2(5) .
O1 Os1 O5 91.19(15) .	O3 C7 C6 114.0(5) .
C11 Os1 O5 174.80(19) .	C8 C7 C6 121.7(5) .
O6 S1 O7 116.7(3) .	C9 C8 C7 125.9(5) .
O6 S1 O5 112.8(3) .	O4 C9 C8 124.6(5) .
O7 S1 O5 113.5(3) .	O4 C9 C10 114.5(5) .
O6 S1 C17 104.3(3) .	C8 C9 C10 120.8(5) .
O7 S1 C17 104.7(4) .	C12 C11 C16 118.6(5) .
O5 S1 C17 103.1(3) .	C12 C11 Os1 121.2(4) .

C16 C11 Os1 120.2(4) .
C11 C12 C13 121.4(6) .
C12 C13 C14 119.2(6) .
C15 C14 C13 119.9(6) .
C14 C15 C16 121.4(6) .
C15 C16 C11 119.5(6) .
F3 C17 F1 127(3) .
F3 C17 F2A 80(3) .
F1 C17 F2A 96(3) .
F3 C17 F1A 116(3) .
F1 C17 F1A 20(3) .
F2A C17 F1A 112.0(13) .
F3 C17 F3A 29(3) .
F1 C17 F3A 118(4) .
F2A C17 F3A 109.0(10) .
F1A C17 F3A 100.1(15) .
F3 C17 F2 98(3) .
F1 C17 F2 97(3) .
F2A C17 F2 22.1(11) .
F1A C17 F2 116.0(18) .
F3A C17 F2 126.4(13) .
F3 C17 S1 118(2) .
F1 C17 S1 111(3) .
F2A C17 S1 116.2(14) .
F1A C17 S1 111.1(13) .
F3A C17 S1 107.0(9) .
F2 C17 S1 96(2) .

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C17 H19 F3 O7 Os S. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Os1	0.01946(11)	0.02288(13)	0.01695(11)	-0.00215(8)	0.00051(8)	-0.00431(8)
S1	0.0219(7)	0.0271(8)	0.0260(7)	-0.0014(6)	-0.0008(6)	0.0007(6)
F1	0.049(13)	0.032(11)	0.16(2)	-0.004(19)	-0.054(17)	-0.015(8)
F2	0.101(16)	0.050(14)	0.116(12)	-0.007(14)	0.015(13)	-0.045(12)
F3	0.096(18)	0.020(8)	0.10(2)	-0.007(13)	-0.037(14)	0.006(8)
F1A	0.057(5)	0.043(6)	0.100(9)	-0.019(6)	-0.045(6)	0.000(4)
F2A	0.076(6)	0.051(7)	0.099(10)	0.009(6)	-0.002(6)	-0.041(5)
F3A	0.068(6)	0.033(5)	0.095(12)	-0.019(6)	-0.019(6)	0.006(4)
O1	0.0226(19)	0.027(2)	0.0201(19)	-0.0029(17)	0.0019(15)	-0.0041(16)
O2	0.027(2)	0.031(2)	0.023(2)	-0.0051(18)	-0.0052(16)	-0.0029(17)
O3	0.0224(19)	0.029(2)	0.0183(18)	-0.0045(17)	-0.0020(15)	-0.0050(16)
O4	0.025(2)	0.028(2)	0.0209(19)	-0.0035(17)	0.0039(16)	-0.0032(17)
O5	0.035(2)	0.034(2)	0.021(2)	0.0040(18)	0.0035(17)	0.0062(19)
O6	0.036(2)	0.048(3)	0.041(3)	0.000(2)	-0.013(2)	0.006(2)
O7	0.041(3)	0.048(3)	0.034(2)	-0.001(2)	0.010(2)	0.002(2)
C1	0.024(3)	0.039(4)	0.035(3)	0.003(3)	0.003(3)	-0.007(3)
C2	0.023(3)	0.020(3)	0.025(3)	-0.001(2)	-0.001(2)	0.000(2)
C3	0.024(3)	0.031(3)	0.031(3)	0.001(3)	-0.010(2)	-0.003(2)
C4	0.034(3)	0.022(3)	0.023(3)	-0.004(2)	-0.004(2)	-0.001(2)
C5	0.037(4)	0.052(4)	0.032(3)	-0.009(3)	-0.005(3)	-0.018(3)
C6	0.029(3)	0.035(4)	0.027(3)	-0.008(3)	-0.003(2)	-0.009(3)
C7	0.021(3)	0.020(3)	0.025(3)	0.003(2)	-0.001(2)	-0.002(2)
C8	0.023(3)	0.035(4)	0.028(3)	0.002(3)	0.002(2)	-0.005(3)
C9	0.022(3)	0.030(3)	0.025(3)	0.002(3)	0.006(2)	0.001(2)
C10	0.038(4)	0.055(4)	0.021(3)	-0.002(3)	0.006(3)	-0.011(3)
C11	0.022(3)	0.022(3)	0.030(3)	-0.001(2)	0.004(2)	-0.003(2)
C12	0.026(3)	0.032(3)	0.031(3)	-0.001(3)	0.005(2)	-0.002(3)
C13	0.030(3)	0.040(4)	0.039(4)	0.011(3)	0.002(3)	-0.001(3)
C14	0.032(3)	0.028(4)	0.059(5)	0.014(3)	0.007(3)	0.003(3)
C15	0.032(3)	0.025(3)	0.048(4)	-0.004(3)	0.014(3)	0.000(3)
C16	0.038(3)	0.031(3)	0.032(3)	-0.008(3)	0.001(3)	-0.007(3)
C17	0.041(4)	0.023(3)	0.098(6)	-0.001(4)	-0.020(4)	-0.001(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for C17 H19 F3 O7 Os S.

	x	y	z	U(eq)
H1A	0.4937	0.6778	0.0290	0.049
H1B	0.6100	0.7703	0.0869	0.049
H1C	0.4677	0.8504	0.0226	0.049
H3	0.5586	0.8131	0.2575	0.035
H5A	0.3597	0.9404	0.4568	0.059
H5B	0.5332	0.8878	0.4209	0.059
H5C	0.4334	0.7818	0.4923	0.059
H6A	-0.1911	0.5318	0.0108	0.045
H6B	-0.3070	0.4376	0.0793	0.045
H6C	-0.1344	0.3708	0.0526	0.045
H8	-0.3188	0.4680	0.2557	0.035
H10A	-0.2015	0.4414	0.4899	0.057
H10B	-0.3608	0.4829	0.4291	0.057
H10C	-0.2758	0.6052	0.4820	0.057
H12	-0.0315	0.8466	0.0667	0.036
H13	-0.2049	1.0505	0.0316	0.045
H14	-0.3203	1.1750	0.1681	0.049
H15	-0.2557	1.0998	0.3353	0.042
H16	-0.0800	0.8993	0.3717	0.040

Computational Details

Electronic energy calculations used the M06[i] hybrid meta functional together with a small-core effective core potential and triple-zeta valence functions of Hay and Wadt[ii] augmented with two f-functions[iii] for Os and the 6-311G**++ basis for other atoms. Geometry optimizations, hessian calculations and solvation energy calculations (at gas-phase geometries) employed the B3LYP functional[iv] with double-zeta contractions of Los Alamos valence functions and 6-31G**[v]. Solvation energies were calculated with the Poisson-Boltzmann reaction field method using a dielectric constant of 2.284 and probe radius of 2.60 to represent the benzene solvent. Jaguar 6.5 and 7.5[vi] were used for all calculations. Reported enthalpies are $H = E_{DFT} + G_{solv} + ZPE + H_{vib} + (12/2)\ kT$, including the electronic energy, free energy of solvation, zero point energy, finite-temperature vibrational energy, and ½ kT for the kinetic and potential energy contributions of the six librational degrees of freedom at T = 140°C. The methyl groups of the acetylacetonate ligands were omitted, which past calculations**Error! Bookmark not defined.** have shown leads to insignificant deviations from calculations using the complete ligand.

Unrestricted wavefunctions were calculated in all cases. Spin-orbit coupling was not included. For Os^{III} intermediates we separately converged three wavefunctions corresponding to the three possible occupations of the quasi-t_2g orbitals by five electrons, and report the lowest energy occupation. No symmetry constraints were employed. All Os^{IV} species were lower in energy as triplets than singlets.

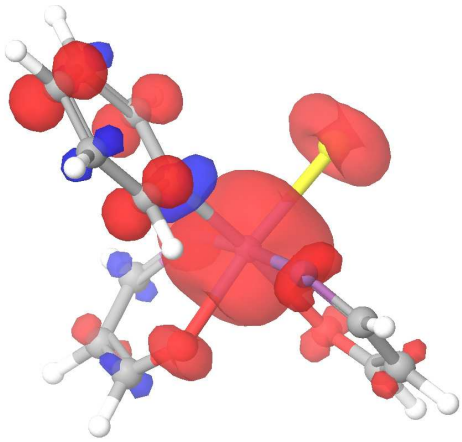


Figure S13. Spin density plot for *cis*-$(acac)_2Os(Ph)(Cl)$ (***cis*-Cl-1-Ph**).

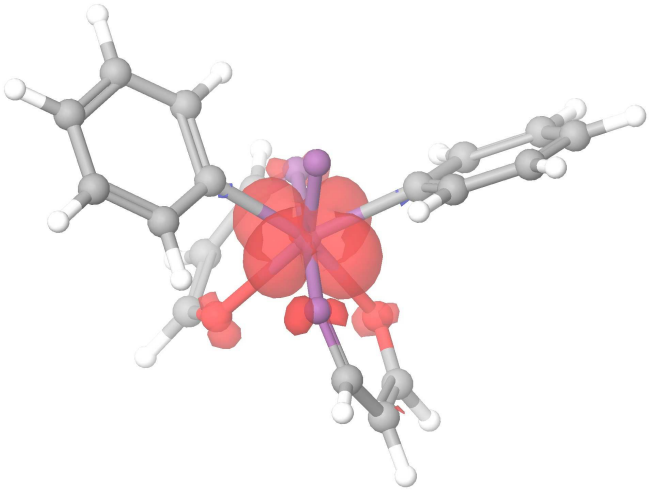


Figure S14. Spin density plot for the CH activation transition state **TS1-H**.

Coordinates and electronic energy in Hartree:

cis-Cl-1-Ph (-1315.7629)

Os1	.7948144975	-.0269922492	.9658202619
O2	.7754693066	1.9979201777	.9607186647
O3	-1.2257013194	.1000525462	.9605477448
C4	-2.0502723118	-.8845078960	.9650585767
C5	-1.7331714519	-2.2394314230	.9969089304
C6	-.4242419904	-2.7262999001	1.0625131094
O7	.6504629618	-2.0333313823	1.0615962193
O8	.5917469199	-.0225273648	3.1813559293
C9	.5316312684	1.0467396468	3.8421031825
C10	.6821719518	2.7387091081	2.0145231136
C11	.5725030524	2.3707363705	3.3452080768
Cl12	3.1154563070	-.0941413234	1.2067737954
C13	.8426166668	-.0610928744	-1.0634023815
C14	1.5050627299	-1.0844203821	-1.7791461188
C15	.1791924974	.9370335842	-1.8127261098
C16	1.5015164353	-1.1104708532	-3.1710954268
C17	.1747525164	.9120498633	-3.2055270651
C18	.8359020546	-.1119174711	-3.8896360446
H19	-3.1028640183	-.5872822762	.9564135229
H20	-2.5462291930	-2.9557543905	1.0038747082
H21	-.2638924459	-3.8058247669	1.1310795086
H22	.4293545262	.9357158046	4.9322638220
H23	.6934460575	3.8088926149	1.7849911267
H24	.5077655854	3.1735603089	4.0713904248
H25	2.0310409934	-1.8611967410	-1.2321582398

H26	-.3294787911	1.7416583763	-1.2909289127
H27	2.0197054381	-1.9061541121	-3.7001937568
H28	-.3410408528	1.6913813047	-3.7609052606
H29	.8338874265	-.1316843047	-4.9763311444

***trans*-Cl-1-Ph (-1315.75914)**

Os1	0.0012382135	-0.0562109954	0.0207839381
O2	-0.1090762224	-0.0769218463	2.0241167597
O3	2.0042107886	-0.0500541656	0.1399810008
C4	2.8130707384	0.1858190008	-0.8261581441
C5	2.4750931283	0.3521980457	-2.1714680278
C6	1.1717308286	0.2555734322	-2.6652222833
O7	0.1113217396	0.0310110367	-1.9809506227
H8	0.9988180762	0.3603078729	-3.7388790244
H9	3.2748375284	0.5410479400	-2.8780260582
H10	3.8631250473	0.2389495506	-0.5291056159
O11	-2.0009099766	0.0040519738	-0.0974908052
C12	-2.8049627269	0.2049725197	0.8804101792
C13	-1.1644790830	0.1350863660	2.7201890646
C14	-2.4646650553	0.2890894540	2.2328050762
H15	-3.8531909811	0.2987505752	0.5870882021
H16	-0.9899922324	0.1770421472	3.7978928470
H17	-3.2604534399	0.4579789804	2.9488176565
Cl18	0.0313896320	2.4323345197	0.0890726210
C20	-0.0234637659	-2.1242082259	-0.0372520511
C21	0.7730453933	-2.8875059770	0.8417566341
C22	0.7584008356	-4.2835835864	0.8039545912

C23	-0.0562805747	-4.9519933601	-0.1170420794
C24	-0.8547870578	-4.2142420428	-0.9984200063
C25	-0.8369161527	-2.8182652448	-0.9573020495
H26	1.4108210030	-2.3820018619	1.5624481958
H27	1.3810984938	-4.8511290150	1.4913254469
H28	-0.0686298324	-6.0383283852	-0.1475083512
H29	-1.4899091745	-4.7277082523	-1.7162202232

Ts1-D (-1087.62816)

Os1	-.6715687001	-.1197727776	-.3726334149
O2	.5657504190	-.2187293115	-1.9959213605
O3	1.1130467799	.1253635032	.8230314520
C4	1.0802303062	.0620260838	2.0865782740
C5	-.0473154006	-.0686006137	2.9185898752
C6	-1.3716794229	-.1224431833	2.4974412412
O7	-1.8417038802	-.0758503091	1.3019978036
H8	-2.1443389949	-.1962055972	3.2702570524
H9	.1299537280	-.0991950845	3.9880642073
H10	2.0570196468	.1320672752	2.5856111986
O11	-.2653098717	-2.1850560350	.1125173285
C12	.6354749273	-2.8430784352	-.4854136594
C13	1.3454546064	-1.2128059373	-2.2327423719
C14	1.4281902141	-2.4351106126	-1.5742731936
H15	.8005402028	-3.8621056386	-.1081623380
H16	2.0122559109	-1.0538310486	-3.0870211085
H17	2.1478085728	-3.1511207047	-1.9558967678
C20	-.5887400189	1.9984677429	-.4174265748

C21	.5364381562	2.6378428745	-.9650382144
C22	.6887619719	4.0211516233	-.8649798672
C23	-.2752149682	4.7960087961	-.2168681573
C24	-1.4014107604	4.1747536909	.3222628135
C25	-1.5614697488	2.7918909852	.2140477837
H26	1.2962626443	2.0518522895	-1.4702978694
H27	1.5693269956	4.4949039909	-1.2922428743
H28	-.1512480197	5.8726885462	-.1378376077
H29	-2.1637545226	4.7656277264	.8240867129
H30	-2.4460149933	2.3209866145	.6328018797
H31	-1.7144976679	.7615930861	-1.1799518098
C40	-2.2593071898	-.9863004156	-1.4761832498
C41	-3.2297756122	-1.7538302600	-.8097931623
C42	-4.1948702302	-2.4615073540	-1.5271423674
C43	-4.2124475792	-2.4214278462	-2.9227904745
C44	-3.2605243718	-1.6562982501	-3.5961230834
C45	-2.3005283949	-.9384409966	-2.8800635814
H46	-3.2301470395	-1.7986979008	.2737997780
H47	-4.9341275559	-3.0518703766	-.9910499080
H48	-4.9632204085	-2.9770498610	-3.4781859741
H49	-3.2654210434	-1.6103204534	-4.6824422070
H50	-1.5681646671	-.3424303553	-3.4166910840

***cis*-(C_6H_6)-2-Ph** (-1087.653209)

Os1	0.1912792634	-0.0494543930	1.0130234328
O2	0.2926398829	2.0145558902	1.0539788585
O3	-1.8063750999	0.3233085751	1.0300914983

C4	-2.7053903157	-0.5772260318	1.1396221631
C5	-2.5190995539	-1.9593142526	1.2436438314
C6	-1.2814467135	-2.6006287400	1.2286213914
O7	-0.1152615462	-2.0780467827	1.1074021492
O8	0.0186304752	-0.0408417218	3.1857422366
C9	-0.3059875152	1.0000089707	3.8329914934
C10	-0.0886156736	2.7224588046	2.0497001402
C11	-0.4013421758	2.3141453193	3.3475070295
C12	0.1994594861	-0.0679152459	-1.0502126730
C13	-0.0863696997	1.1025016991	-1.7891308617
C14	0.4505311909	-1.2387780695	-1.8004288192
C15	-0.0910086702	1.1092070002	-3.1835840735
C16	0.4297164428	-1.2419203344	-3.1960866427
C17	0.1668488783	-0.0640741626	-3.8964991923
H18	-3.7293016783	-0.1889391019	1.1511234294
H19	-3.4039737601	-2.5788149241	1.3386142223
H20	-1.2727789749	-3.6918996414	1.3224831130
H21	-0.5172903213	0.8500564028	4.9023943575
H22	-0.1378619443	3.7971113795	1.8364770096
H23	-0.6865057781	3.0882325977	4.0519407332
H24	-0.2909591727	2.0256082154	-1.2551673893
H25	0.6373807565	-2.1751580507	-1.2804323423
H26	-0.3020864073	2.0331803312	-3.7175077909
H27	0.6198886191	-2.1664857650	-3.7366642867
H28	0.1575902036	-0.0607174460	-4.9834037171
C29	2.5856645318	0.3858055798	0.9019072172
C30	2.4132919420	-1.0168644642	0.9623559011

C31	3.0685153677	1.0760227596	2.0546508926
C32	2.7212854254	-1.7078830100	2.1727896000
C33	3.3477276391	0.3873598365	3.2116302218
C34	3.1701641382	-1.0187625145	3.2737211547
H35	2.5729386920	0.8970403517	-0.0535870121
H36	2.2866746098	-1.5854879849	0.0502683104
H37	3.2308041747	2.1477799370	1.9979472782
H38	2.6020808354	-2.7860838888	2.2056554746
H39	3.7200340101	0.9186849455	4.0836045597
H40	3.4006699676	-1.5484829216	4.1938007812

***trans*-(C_6H_6)-2-Ph (-1087.65743)**

Os1	-0.0068964751	0.1170726025	-2.3778384779
O2	0.2373085720	2.1288273120	-2.1344074627
O3	-1.9790112506	0.5026542649	-2.7143954361
C4	-2.8637561473	-0.4173703552	-2.8232976279
C5	-2.6580725538	-1.8002098525	-2.8458762357
C6	-1.4094452576	-2.4296166315	-2.8292394918
O7	-0.2572156863	-1.8789934098	-2.7325157889
O8	1.9903985438	-0.2755686168	-2.2189392106
C9	2.8610331625	0.6533114898	-2.0657277864
C10	1.3893773471	2.6668728313	-1.9842623100
C11	2.6366223773	2.0300493832	-1.9516727006
C12	-1.1265526467	0.7397525554	0.3370109745
C13	-1.3282848757	0.5578054987	1.7056673585
C14	-0.7160510052	-0.5050065432	2.3738822633
C15	0.1031611924	-1.3850403950	1.6631310050

C16	0.3072466414	-1.2075997627	0.2943223802
C17	-0.3113859273	-0.1459080284	-0.3960867475
H18	-3.8891220628	-0.0490935109	-2.9382835940
H19	-3.5331473981	-2.4323103401	-2.9524881039
H20	-1.3839048902	-3.5193685536	-2.9413161608
H21	3.8970651023	0.3001459635	-2.0191733961
H22	1.3703658142	3.7565619750	-1.8709965977
H23	3.5078145432	2.6606796548	-1.8087888003
H24	-1.6000610662	1.5739216635	-0.1717197677
H25	-1.9621370093	1.2512668900	2.2534047660
H26	-0.8712247761	-0.6428307514	3.4408050646
H27	0.5894101455	-2.2107565825	2.1773839265
H28	0.9524782370	-1.8920534927	-0.2478968843
C29	-1.3315864366	1.1716483103	-6.4553793340
C30	-0.3005232289	1.8162967944	-5.7759632211
C31	0.7672904529	1.0735639698	-5.2555208830
C32	0.7943897407	-0.3178852104	-5.4131160932
C33	-0.2445951660	-0.9615774420	-6.0976085751
C34	-1.3019193237	-0.2181181405	-6.6182030689
H40	-2.1597535451	1.7477213152	-6.8586999864
H35	-0.3228082917	2.8943307840	-5.6463938561
H36	1.5894460839	1.5801330045	-4.7584366761
H37	1.6247484999	-0.8935551954	-5.0171010781
H38	-0.2216978800	-2.0402799139	-6.2220683087
H39	-2.1066111520	-0.7184349961	-7.1501820248

***cis*-3 (-2171.315099)**

Os1	0.2893427480	2.1042011400	-0.1699188180
O2	0.6969509783	2.8324705634	-2.0248679647
O3	-1.7788084475	2.5962368057	-0.5446076252
C4	-2.7248026342	2.4249090571	0.2855590078
C5	-2.6298263226	1.8797807911	1.5743216157
C6	-1.4487843799	1.4239728755	2.1559820614
O7	-0.2680668659	1.4324735041	1.6575380003
O8	0.4470851291	3.9389549019	0.7096363175
C9	0.7255710859	4.9982542153	0.0508062252
C10	0.9296358074	4.0745394797	-2.2450495696
C11	0.9709286006	5.1199199677	-1.3212172091
Cl12	0.0000000000	0.0000000000	-1.3456665788
C47	2.2677150142	1.7693986922	0.2331894855
C48	2.8032342326	2.0864968705	1.5023615130
C49	3.1693847516	1.2797117631	-0.7390665542
C50	4.1576005963	1.9163861699	1.7877684850
C52	4.5276429168	1.1232629479	-0.4616695301
C54	5.0285479094	1.4370144864	0.8050418037
H13	-3.7187198056	2.7450713562	-0.0551460199
H14	-3.5419714799	1.7803041619	2.1508211017
H15	-1.4997581618	0.9986339226	3.1628033413
H16	0.7603605983	5.9071143128	0.6608241839
H17	1.1128743550	4.3133750102	-3.2976385930
H18	1.1894759244	6.1116455832	-1.7010450554
H51	2.1413033140	2.4690950250	2.2743003031
H53	2.7990841088	1.0274899261	-1.7286757758
H55	4.5382459164	2.1657991464	2.7757324374

H56	5.1975286463	0.7540099375	-1.2348161021
H57	6.0865230829	1.3139765742	1.0225734849
Os19	-0.2893427480	-2.1042011400	-0.1699188180
O20	0.2680668659	-1.4324735041	1.6575380003
O21	-0.4470851291	-3.9389549019	0.7096363175
C22	-0.7255710859	-4.9982542153	0.0508062252
C23	-0.9709286006	-5.1199199677	-1.3212172091
C24	-0.9296358074	-4.0745394797	-2.2450495696
O25	-0.6969509783	-2.8324705634	-2.0248679647
O26	1.7788084475	-2.5962368057	-0.5446076252
C27	2.7248026342	-2.4249090571	0.2855590078
C28	1.4487843799	-1.4239728755	2.1559820614
C29	2.6298263226	-1.8797807911	1.5743216157
C30	-2.2677150142	-1.7693986922	0.2331894855
C31	-3.1693847516	-1.2797117631	-0.7390665542
C32	-2.8032342326	-2.0864968705	1.5023615130
C33	-4.5276429168	-1.1232629479	-0.4616695301
C34	-4.1576005963	-1.9163861699	1.7877684850
C35	-5.0285479094	-1.4370144864	0.8050418037
H36	-0.7603605983	-5.9071143128	0.6608241839
H37	-1.1894759244	-6.1116455832	-1.7010450554
H38	-1.1128743550	-4.3133750102	-3.2976385930
H39	3.7187198056	-2.7450713562	-0.0551460199
H40	1.4997581618	-0.9986339226	3.1628033413
H41	3.5419714799	-1.7803041619	2.1508211017
H42	-2.7990841088	-1.0274899261	-1.7286757758
H43	-2.1413033140	-2.4690950250	2.2743003031

H44	-5.1975286463	-0.7540099375	-1.2348161021
H45	-4.5382459164	-2.1657991464	2.7757324374
H46	-6.0865230829	-1.3139765742	1.0225734849

***Cis*-2-Ph (-855.4963201)**

Os1	0.6748421521	-0.0641510912	0.9284481455
O2	0.8097692123	1.9888206304	0.9760463014
O3	-1.2707901450	0.1322533323	1.2053290843
C4	-2.0231657045	-0.8940123868	1.4236898798
C5	-1.6622659469	-2.2389774558	1.4727207441
C6	-0.3734776326	-2.7498821823	1.2784267511
O7	0.6892449207	-2.0803585681	1.0163460299
O8	0.8562219621	-0.0411463982	3.0897949176
C9	0.6974553484	1.0010920671	3.8000737011
C10	0.6466638298	2.7202309822	2.0137180815
C11	0.5469073013	2.3196989146	3.3478480944
C13	0.8063684586	-0.0110217091	-1.0972899642
C14	1.4847387778	-1.0493119079	-1.7808730127
C15	0.3231222785	1.0640560975	-1.8816142880
C16	1.6896190819	-1.0047755041	-3.1614134958
C17	0.5173978332	1.1061462280	-3.2584133728
C18	1.2058291338	0.0721900914	-3.9042132248
H19	-3.0715040181	-0.6250416451	1.5754252486
H20	-2.4540033872	-2.9527590895	1.6724975475
H21	-0.2284717133	-3.8321033224	1.3433029186
H22	0.7104705451	0.8416266590	4.8878277330
H23	0.6251297950	3.7959785050	1.8037743069

H24	0.4305114174	3.0979328137	4.0941481751
H25	1.8400242428	-1.9119858562	-1.2222006006
H26	-0.2006081343	1.8792318476	-1.3905430134
H27	2.2163358846	-1.8161249623	-3.6580116117
H28	0.1343693613	1.9442051958	-3.8358618700
H29	1.3562220547	0.1055714470	-4.9801850803

$(acac)_2Os(IV)(C_6H_6)(C_6H_5)^+[Cl^-]$ (42.6 kcal/mol) (-1547.808482)

Os1	-0.4066894646	-0.2477540961	-0.4483168903
O2	1.0615374800	-0.3633415768	-1.8810801266
O3	1.1890783036	0.0341445580	0.9881131718
C4	1.0522714539	-0.2136261529	2.2254835626
C5	-0.1399757177	-0.5010527687	2.9080653673
C6	-1.4114422798	-0.4965881330	2.3336213779
O7	-1.7307743071	-0.2812627250	1.1119046517
H8	-2.2709246622	-0.6622061477	2.9920734579
H9	-0.0785235570	-0.6782895923	3.9761814028
H10	1.9742884313	-0.1737857928	2.8226913437
O11	-0.1977311872	-2.2328047850	0.0079649063
C12	0.7101129987	-2.9848995523	-0.4759759571
C13	1.7926933338	-1.4082224611	-2.0470831782
C14	1.6826651182	-2.6490136255	-1.4267527102
H15	0.6982871210	-4.0092118222	-0.0879785950
H16	2.5878030607	-1.2791506341	-2.7890671567
H17	2.3882356163	-3.4197201197	-1.7160160852
C20	-1.2134287539	2.0960136075	-0.3733904261
C21	-0.2773330158	1.9983936503	-1.4267345984

C22	1.0262570229	2.5525665785	-1.2646677061
C23	1.3756112500	3.1684024576	-0.0850618580
C24	0.4398872005	3.2656953408	0.9740256686
C25	-0.8266946037	2.7418919170	0.8364580106
H26	-0.6108322997	1.7127612381	-2.4175436545
H27	1.7320649944	2.4904199509	-2.0863773150
H28	2.3683562346	3.5929312711	0.0358110569
H29	0.7231988684	3.7709414200	1.8936356390
H30	-1.5571129370	2.8420447842	1.6333547595
H31	-2.2630726026	1.8740433838	-0.5448824236
Cl32	-4.6532875818	1.3101684678	-1.0105333148
C40	-1.9156973023	-0.6630114358	-1.7681555146
C41	-3.2409318993	-0.9757274076	-1.3229948282
C42	-4.2304283628	-1.4455230764	-2.2197030507
C43	-3.9433342003	-1.5892341762	-3.5647052328
C44	-2.6610028270	-1.2516788389	-4.0272614710
C45	-1.6752813585	-0.7986313206	-3.1506528772
H46	-3.4437012262	-0.9873694909	-0.2599811367
H47	-5.2188063018	-1.6739927363	-1.8347024362
H48	-4.6999478330	-1.9441695699	-4.2577099426
H49	-2.4305375338	-1.3422484150	-5.0864536960
H50	-0.6922351559	-0.5639297345	-3.5470674077

$(acac)_2Os(IV)(C_6H_5)(H)(C_6H_5)^+[Cl^-]^‡$ (61.6 kcal/mol) (-1547.768607)

Os1	-0.4019347622	-0.2372392802	-0.4707358319
O2	0.9797088504	-0.3825551517	-1.9649382946
O3	1.2432319079	-0.0077841850	0.8800464003

C4	1.1189220336	-0.1095752218	2.1366070528
C5	-0.0707044523	-0.2827294617	2.8691883314
C6	-1.3512848758	-0.2883283771	2.3306792252
O7	-1.7041008330	-0.1630980668	1.0982153271
H8	-2.1956427401	-0.3753321261	3.0216732919
H9	0.0144815406	-0.3599170169	3.9473147243
H10	2.0531779552	-0.0339559039	2.7085621197
O11	-0.0987323884	-2.2988790890	0.0175499155
C12	0.8586566078	-2.9815711830	-0.4536753720
C13	1.8028858825	-1.3655087919	-2.0876782972
C14	1.8062167823	-2.5807931261	-1.4146282915
H15	0.9355076566	-4.0082033160	-0.0719401423
H16	2.5685376356	-1.2031926575	-2.8528461126
H17	2.5678594979	-3.3001616388	-1.6937280460
C20	-0.5228780100	1.8505271822	-0.7837867864
C21	0.3678863126	2.4985391074	-1.6713967139
C22	0.4965567183	3.8814663122	-1.6599585667
C23	-0.2772817590	4.6557348096	-0.7884198020
C24	-1.1972373468	4.0375894942	0.0610727032
C25	-1.3346907153	2.6539047534	0.0512952749
H26	0.9644276865	1.9044354726	-2.3534292330
H27	1.1958245515	4.3626783585	-2.3382087891
H28	-0.1768951753	5.7375522227	-0.7879443123
H29	-1.8231811809	4.6367486513	0.7161072899
H30	-2.0742421153	2.1811004818	0.6872583767
H31	-1.4075534446	0.7142707786	-1.4240078038
Cl32	-3.0107231019	2.2308190413	-2.9131529451

C40	-2.0011076791	-0.7026617421	-1.7765176669
C41	-3.2967066871	-0.9548271873	-1.2688454719
C42	-4.2699318110	-1.5395189067	-2.0695185780
C43	-3.9899554853	-1.8610854978	-3.4020181745
C44	-2.7306151055	-1.5752570180	-3.9350162114
C45	-1.7534519522	-0.9857925058	-3.1401609280
H46	-3.5229092868	-0.6997080703	-0.2404771739
H47	-5.2560803591	-1.7374784096	-1.6589472511
H48	-4.7565289890	-2.3114505324	-4.0261560946
H49	-2.5176003805	-1.7919958056	-4.9779449704
H50	-0.7904873227	-0.7327439827	-3.5690366014

(κ^2-acac)(κ^1-acac)Os(IV)(Cl)(C_6H_5)(C_6H_6) (22.4 kcal/mol) (-1547.841477)

Os1	0.0059025213	-0.0021592116	-0.0046049631
O2	0.0199257097	0.0106251398	1.9422289244
O3	2.1799550797	-0.0046891364	-0.0706901767
C4	2.8831904444	0.2216921711	-1.0939403609
C5	2.4166812170	0.3166539835	-2.4223194302
C6	1.0970169615	0.1141445910	-2.7907897613
O7	0.0875434842	-0.1235477870	-2.0214041776
H8	0.8423164850	0.1325326060	-3.8547369558
H9	3.1392293874	0.5120170898	-3.2064795269
H10	3.9632273119	0.3326045070	-0.9239324645
O11	0.3921895924	-1.6011126679	4.3005519910
C12	0.1625639986	-0.5219234129	4.8363866324
C13	-0.1820944282	0.9587923868	2.8330517333
C14	-0.1243977417	0.7457727250	4.1794122085

H15	0.1661403936	-0.4566960611	5.9474318772
H16	-0.3965192798	1.9531101684	2.4368158273
H17	-0.3037033346	1.6033064264	4.8211126259
H18	-1.1250823946	-2.3590129524	0.7258023722
C18	-2.0504376235	0.0218723302	-0.1039137947
C19	-2.8514393041	-0.4746177673	0.9465066100
C20	-4.2450943036	-0.4758311198	0.8615745035
C21	-4.8804427968	0.0193203286	-0.2770107607
C22	-4.1074346309	0.5273767255	-1.3235516083
C23	-2.7162301766	0.5385982993	-1.2336088113
H24	-2.3834463111	-0.8478509211	1.8538434731
H25	-4.8327987205	-0.8623067267	1.6907007502
H26	-5.9648930307	0.0164807624	-0.3462999985
H27	-4.5907358118	0.9249893331	-2.2128739518
H28	-2.1351235296	0.9448835112	-2.0547121137
Cl30	0.0732501798	2.3362465997	-0.1910324879
C31	-0.1353744212	-2.5461982321	0.3234307355
C32	0.9591828021	-2.6969000072	1.2052751731
C33	2.1670343809	-3.1961993089	0.7220232244
C34	2.2851639634	-3.5616074217	-0.6210533233
C35	1.2058076439	-3.4224007215	-1.5021220859
C36	-0.0067915344	-2.9296884511	-1.0312551177
H37	0.8452337171	-2.4046029619	2.2456849147
H38	3.0145263815	-3.3035667987	1.3919851686
H39	3.2288285412	-3.9554050712	-0.9901795377
H40	1.3120359311	-3.7107709265	-2.5436656718
H41	-0.8599264766	-2.8303189162	-1.6945668302

(κ^2-acac)(κ^1-acac)Os(IV)(Cl)(C_6H_5)(H)(C_6H_5)‡ (62.5 kcal/mol) (-1547.771852)

Os1	0.0228146992	-0.0338839174	-0.0049944846
O2	0.0430398843	-0.0296652188	2.0054776379
O3	2.0937437234	-0.0448561594	-0.0728878444
C4	2.7793392575	0.2671027931	-1.0970096017
C5	2.3109811776	0.4537865100	-2.4051714164
C6	0.9986311442	0.2163064479	-2.8032110918
O7	0.0035761543	-0.1279039989	-2.0699902208
H8	0.7628614048	0.2877712512	-3.8702566649
H9	3.0321613474	0.7192523149	-3.1692103358
H10	3.8546475949	0.3638550509	-0.9136819867
O11	2.5912288622	2.3135043223	1.1393986206
C12	2.2284956940	2.5482087499	2.2806636678
C13	0.4459766516	0.7486103475	2.9851155375
C14	1.2949068348	1.8137112706	3.1333143382
H15	2.6585421331	3.4259311642	2.8179508894
H16	-0.0394822802	0.4420812342	3.9195323226
H17	1.2896565386	2.1928075305	4.1539477290
H18	-1.1286557352	-1.4333126638	0.1391034523
C18	-2.1392808235	-0.4282463750	0.0706277290
C19	-2.8428157156	-0.3472897953	1.2861301539
C20	-4.2326321252	-0.2513093157	1.2919644216
C21	-4.9384585230	-0.2532380233	0.0868302233
C22	-4.2531760829	-0.3611256830	-1.1260404515
C23	-2.8640042405	-0.4585965614	-1.1358350136
H24	-2.2882401136	-0.3535029169	2.2173421494

H25	-4.7660165772	-0.1754719924	2.2355375686
H26	-6.0225241667	-0.1783117071	0.0925158951
H27	-4.8026821202	-0.3670377856	-2.0633463318
H28	-2.3304340143	-0.5350928898	-2.0770701491
Cl30	-0.3658936299	2.2932459728	-0.1889719722
C31	0.0694459653	-2.2424690843	0.0656398165
C32	0.4336689050	-2.8735608773	1.2693068996
C33	0.8302212995	-4.2097435655	1.2726201153
C34	0.8441723353	-4.9401054279	0.0822132859
C35	0.4523503236	-4.3344818564	-1.1143493258
C36	0.0600901267	-2.9975502134	-1.1217454345
H37	0.4139069623	-2.3045689070	2.1914938192
H38	1.1254585554	-4.6833147962	2.2050197420
H39	1.1505545946	-5.9826934313	0.0881459705
H40	0.4505420655	-4.9053780919	-2.0389233104
H41	-0.2536748671	-2.5298263663	-2.0492161698

***trans*-(acac)$_2$Os(C6H5)(OTf) (*trans*-OTf-1-Ph) (-1817.00189)**

Os1	0.2243301246000	-0.1456765492000	-0.0443638613000
O2	0.2050927079000	-0.0965708493000	1.9535281593000
O3	2.2120271763000	-0.3244581252000	-0.0262226559000
C4	3.0153447515000	-0.1040094480000	-0.9999826454000
C5	2.6452050235000	0.1268555589000	-2.3287974881000
C6	1.3224004974000	0.1361672219000	-2.7672846677000
O7	0.2758235806000	-0.0384708322000	-2.0385810463000
H8	1.1071217322000	0.2914364609000	-3.8262638146000
H9	3.4287506368000	0.2937865513000	-3.0581194247000

H10	4.0712129886000	-0.1201100033000	-0.7252571581000
O11	-1.7552374543000	0.1653733687000	-0.0631210205000
C12	-2.5019358371000	0.4143300673000	0.9504038728000
C13	-0.7956301359000	0.1812163920000	2.7088975320000
C14	-2.1032028108000	0.4298532526000	2.2887568650000
H15	-3.5436548623000	0.6248212838000	0.6986722685000
H16	-0.5555399291000	0.2167980555000	3.7733342582000
H17	-2.8480403857000	0.6566885334000	3.0423134013000
O18	0.3121320817000	2.0853848824000	-0.0983053323000
C20	-0.0205857582000	-2.1707268476000	-0.0492571514000
C21	0.7601543242000	-2.9985991669000	0.7861953317000
C22	0.5865516202000	-4.3829521640000	0.7880026013000
C23	-0.3710688227000	-4.9713517175000	-0.0466053268000
C24	-1.1536364917000	-4.1672163908000	-0.8833565667000
C25	-0.9807791675000	-2.7824075380000	-0.8837393341000
H26	1.5072727410000	-2.5526088403000	1.4369087565000
H27	1.1968496163000	-5.0040276175000	1.4383960353000
H28	-0.5064105540000	-6.0493468297000	-0.0443695055000
H29	-1.8976294873000	-4.6203198166000	-1.5331585984000
H30	-1.5946358753000	-2.1677860508000	-1.5363178655000
S31	1.3910748362483	3.1250094833831	0.2276631052106
O32	2.6583103017644	2.5248230353162	0.6654586927074
O33	1.4217320721053	4.2063324570248	-0.7578492421647
C34	0.6662042242228	3.9032833515942	1.7762864842891
F35	1.4741120615222	4.8696206114986	2.2333987920450
F36	0.5231860538109	2.9783814271854	2.7511264895633
F37	-0.5425645673387	4.4356286211735	1.5318880796204

***cis*-(acac)$_2$Os(C_6H_5)(OTf) (*cis*-OTf-1-Ph) (-1816.993337)**

Os1	-0.4585437330000	0.0111482751000	-0.3412776876000
O2	1.0759826477000	-0.0322774438000	-1.6337246088000
O3	0.8800050712000	0.2106458244000	1.1517969657000
C4	0.6062479963000	0.2968770558000	2.4036951906000
C5	-0.6595783137000	0.2471469170000	2.9907663141000
C6	-1.8428799756000	0.0510926464000	2.2735470878000
O7	-1.9527286633000	-0.0685859680000	1.0018767969000
H8	-2.7895254992000	-0.0214951123000	2.8146609086000
H9	-0.7248587171000	0.3308522081000	4.0693680424000
H10	1.4850093332000	0.4011464428000	3.0449049796000
O11	-0.2302315419000	-2.1714721026000	-0.0976238542000
C12	0.5544292175000	-2.8743945362000	-0.7933446427000
C13	1.6433214207000	-1.0847349595000	-2.1315285829000
C14	1.4480897166000	-2.4129158623000	-1.7881745883000
H15	0.5428940820000	-3.9544716970000	-0.5913227174000
H16	2.3760754952000	-0.8483169658000	-2.9063971814000
H17	2.0395586620000	-3.1537893411000	-2.3147536197000
O18	-1.8096034220793	-0.4736588587488	-1.7791114840365
C20	-0.6087510946825	2.0259450570031	-0.5328599468108
C21	0.5542747711747	2.8301534619809	-0.6170876324680
C22	0.4651084976888	4.2167126883683	-0.7113110356858
C23	-0.7906696645987	4.8395019340899	-0.7232938500377
C24	-1.9541690107756	4.0651499122367	-0.6443398309346
C25	-1.8655495033150	2.6772506042467	-0.5543065821839
H26	1.5304617029173	2.3548769280101	-0.6183600618397

H27	1.3695484421988	4.8155278010354	-0.7794910499918
H28	-0.8606113739558	5.9212466950372	-0.7994092970534
H29	-2.9293430154199	4.5437691361529	-0.6663922023811
H30	-2.7761102239790	2.0885425316390	-0.5127199384704
S31	-2.0056472178624	0.0127572488899	-3.2589685639740
O32	-2.6305228778492	1.3284071157303	-3.3456970205338
O33	-0.8523419867811	-0.3102303332898	-4.0974000446292
C34	-3.3467676117999	-1.2299431592072	-3.6965602407254
F35	-3.7524846792491	-0.9964563559913	-4.9526039912619
F36	-4.3959373942298	-1.1047619615110	-2.8733096367969
F37	-2.8779254947051	-2.4834393084532	-3.6184320577003

$[Os(acac)_2(C_6H_5)(C_6H_6)](C_6H_6)$ (-1319.76790) (associative substitution precursor)

Os	0.056910119	-0.9328663018	1.2560790841
O	1.078475976	0.8597751653	1.4748429774
O	-1.414652528	0.3099109064	0.6210324206
C	-2.576676237	-0.0840166428	0.2629877839
C	-3.064873461	-1.3943677018	0.2393134486
C	-2.350189696	-2.5221411682	0.6459575096
O	-1.142343857	-2.5875785081	1.0712430285
O	-0.751334991	-0.6670521314	3.2707738715
C	-0.712001623	0.4525137597	3.8722158148
C	0.8041935708	1.7347783968	2.3639633914
C	-0.0255520208	1.6106571285	3.4846394967
C	0.6889490007	-1.1013701511	-0.6854694584
C	0.9425169293	0.0666332125	-1.4455663086
C	0.7923474083	-2.3328134239	-1.3718461454

C	1.3062197444	0.0087377132	-2.7891178401
C	1.1402781958	-2.3958159054	-2.7214590229
C	1.4076176257	-1.2263897569	-3.4357680592
H	-3.2470388494	0.7247660301	-0.0466264592
H	-4.0867940893	-1.5412793942	-0.0962203233
H	-2.8638121063	-3.4885689657	0.6129959003
H	-1.2734788626	0.5033307281	4.8157453202
H	1.3308625363	2.6880204383	2.2232548922
H	-0.1027621067	2.4766066785	4.1333615334
H	0.8424576794	1.0375028224	-0.9682322574
H	0.5748208130	-3.2529131125	-0.8431386465
H	1.4992391352	0.9287494997	-3.3395442439
H	1.1977984529	-3.3602965955	-3.2202592576
H	1.6794976119	-1.2742208751	-4.4870687199
C	2.9907809764	3.6319030947	0.0424438388
C	4.0042657486	3.8674114212	0.9745311343
C	2.2689924502	4.7056251740	-0.4842669710
C	4.2971932094	5.1720919543	1.3768442873
C	2.5613719133	6.0100649400	-0.0821367425
C	3.5760151392	6.2437178705	0.8481016198
H	2.7601250182	2.6150596341	-0.2629607573
H	4.5669961288	3.0331394242	1.3844202970
H	1.4791594268	4.5249801916	-1.2078562096
H	5.0858746340	5.3539880249	2.1010575157
H	1.9998525215	6.8446350597	-0.4926268553
H	3.8044749070	7.2590850968	1.1608104813
C	2.7579085398	-3.8690625137	0.8597703435

C	3.5991639626	-2.7301489728	0.8361753649
C	3.2896978384	-1.6222076555	1.5913245547
C	2.1179312128	-1.6109018768	2.4007578808
C	1.2735326825	-2.7436979012	2.4170088499
C	1.6166474556	-3.8778276913	1.6293652957
H	3.0195229405	-4.7388000973	0.2661930730
H	4.4960340131	-2.7385527360	0.2234537107
H	3.9405978332	-0.7543525202	1.5937680847
H	2.0185113053	-0.8473833545	3.1651748975
H	0.5057502235	-2.8403848338	3.1760261562
H	0.9751870133	-4.7524924342	1.6591430548

TS-3 Os(acac)$_2$(ph)(bz)(bz) (-1319.73647069561) (associative substitution TS)

Os	-0.221698965	-0.3331349958	0.7608875515
O	-0.005735504	1.7078428147	0.9067005452
O	-2.173059164	-0.0464143797	0.8360372790
C	-2.990906951	-1.0433239908	0.9112474861
C	-2.699635360	-2.4060351207	0.9223245723
C	-1.421412105	-2.9733632676	0.8457056812
O	-0.306766559	-2.3469035864	0.7460596353
O	-0.216833011	-0.4042640070	2.9275260785
C	-0.348801978	0.6216578590	3.6737493809
C	-0.1701658733	2.4071297505	1.9623013090
C	-0.3776424726	1.9607571060	3.2724217024
C	0.0656457682	-0.1945200282	-1.2464107689
C	-0.3696668269	0.9114628610	-2.0152744910
C	0.7920739482	-1.2018330979	-1.9260503716

C	-0.0849990649	1.0121372508	-3.3740263238
C	1.0873383011	-1.0991012656	-3.2871163838
C	0.6494405916	0.0073588424	-4.0153775908
H	-4.0361310955	-0.7287469882	0.9646466026
H	-3.5412059653	-3.0867448189	0.9913139487
H	-1.3338374840	-4.0635959696	0.8644169392
H	-0.4191488096	0.4161790049	4.7509981283
H	-0.0967570417	3.4881875081	1.7993666425
H	-0.4799653739	2.7153133975	4.0446554902
H	-0.9297340937	1.7038005993	-1.5261957854
H	1.1138205288	-2.0866391068	-1.3812883906
H	-0.4346673275	1.8722730348	-3.9404415970
H	1.6487208246	-1.8883935713	-3.7813386799
H	0.8701930394	0.0859655511	-5.0768520643
C	3.7094461335	1.6748770746	0.4193702858
C	4.3603402980	1.9540639703	1.6238550384
C	3.0073157277	2.6824402531	-0.2465323213
C	4.3108072777	3.2414636454	2.1632064495
C	2.9632251552	3.9705050283	0.2908059100
C	3.6137479369	4.2501893137	1.4949754286
H	3.7472388011	0.6736146371	-0.0015951475
H	4.9065444783	1.1704976964	2.1427683825
H	2.4862910386	2.4584738276	-1.1723919939
H	4.8153809925	3.4583554605	3.1009792487
H	2.4196499457	4.7559104990	-0.2279577339
H	3.5776532832	5.2532228271	1.9123726478
C	3.8700681216	-4.4395533743	3.0133016541

C	4.7801232912	-3.5290098166	2.4721822729
C	4.4190613987	-2.1883477455	2.3227488822
C	3.1485003756	-1.7593271188	2.7139406594
C	2.2356685880	-2.6704422299	3.2521437878
C	2.5994002506	-4.0101134718	3.4021811643
H	4.1510975184	-5.4829794683	3.1305193555
H	5.7684320918	-3.8635586714	2.1681869664
H	5.1289641404	-1.4803170306	1.9021414594
H	2.8702561529	-0.7136631494	2.6080761797
H	1.2469082856	-2.3269020423	3.5385933617
H	1.8915903782	-4.7208544495	3.8211964586

TS-2 (-1315.713759)

Os1	0.5331332978	0.0438052643	0.5217975075
O2	0.4572142137	2.1112711823	0.6046042363
O3	-1.5052606165	0.0713024618	0.5555906648
C4	-2.2198620980	-0.9837298801	0.6960669862
C5	-1.8116103682	-2.3054190282	0.8394261225
C6	-0.4761687994	-2.7435826230	0.8504874359
O7	0.5755850061	-2.0563784039	0.6981478514
O8	0.4720198991	-0.1205612579	2.5638561135
C9	0.4836105451	0.8949214119	3.3456155354
C10	0.4551426434	2.7575819473	1.7039009143
C11	0.4884315838	2.2477039534	3.0076390518
C12	0.8413880309	0.6270194662	-1.7154411784
C13	1.6603686794	-0.3681480572	-1.1020851774
C14	1.9537027961	-1.6107840890	-1.7353480893

C15	1.2599314367	-1.9213338973	-2.8767939743
C16	0.3207468470	-1.0140343677	-3.4491872716
C17	0.1356916196	0.2284587087	-2.8984002581
H19	-3.2966430818	-0.7793431356	0.7070506998
H20	-2.5845023661	-3.0553337361	0.9656269381
H21	-0.3047790523	-3.8181313410	0.9993279866
H22	0.4797882226	0.6354411144	4.4103956665
H23	0.4168284669	3.8465218437	1.5858911903
H24	0.4898753427	2.9639422516	3.8216215037
H25	0.9673894034	1.6834748270	-1.5141259699
H26	2.6510084235	-2.3020315325	-1.2787930469
H27	1.4207965862	-2.8877283884	-3.3475362599
H28	-0.2058873179	-1.2957700890	-4.3560071433
H29	-0.4935447111	0.9630070747	-3.3936669694
Cl18	3.0865631763	0.2956695068	0.2037800279

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